Radiative Transfer in Entry Flows

10th International Planetary Probe Workshop, EDL Short Course San José, California, 15–21 June 2013

M. Lino da Silva¹ and Lionel Marraffa²

 Instituto de Plasmas e Fusão Nuclear Instituto Superior Técnico, Lisboa, Portugal
 ESA-ESTEC, Aerothermodynamics Section Noordwijk, The Netherlands

15 June 2013



Introduction

- Radiative heating can be a major design driver for large or high-speed ($\geq 10 km/s$) entry vehicles
- For lower entry speeds, radiative heating may mandate additional thermal protections (e.g. base heating for Martian entries)
- Convective heating mostly depends on ground species, radiative heating depends on excited species.
 Larger uncertainties
- Accounting for an additional spectral dimension with grids with over 10⁶ points. Very computationally intensive CFRD simulations.



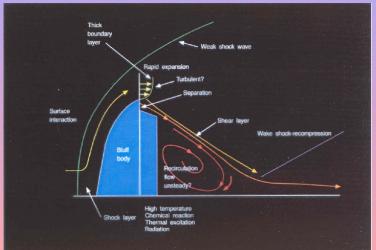


Main Drivers

- Do we need to take radiation into account?
- Optically thin or thick?
- Coupling between flow and radiation?
- Equilibrium or non-equilibrium radiation?
- Selection of an appropriate radiative database
- Other issues (precursor, photo-chemistry, photo-ionisation processes)



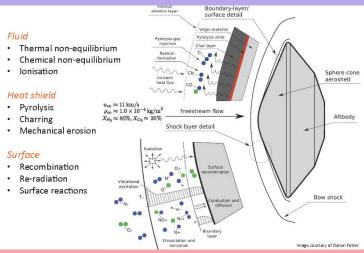
Aerothermodynamics of Entry Vehicles







Aerothermodynamics of Entry Vehicles







Engineering Correlations for Radiation

- Engineering Correlations useful when exploring different EDL scenarios
- Exploratory paameters: Spacecraft sizing, atmospheric profiles and composition, entry path and angle, aerodymamic coefficients, etc...
- Correlations then complemented with detailed CFRD calculations for pre-selected Flight pathss, at specific representative entry points (\sim 5)





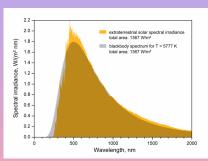
Blackbody radiation limit

spectral emissivity of a gas has a theoretical limit given by Planck's law

$$B_{\nu}(T) = \frac{2h\nu^3}{c^2} \left[exp\left(\frac{h\nu}{k_BT}\right) - 1 \right]^{-1}$$

The spectral integration yields the Stefan–Boltzmann Law:

$$\int_{\mathcal{U}} B_{\nu}(T) = \sigma T^4$$



The Sun's emissivity is close to a blackbody



Engineering correlations are based on this upper theoretical limit for the emitted radiation



Stagnation Streamline flux dependence on cone radius

Convective fluxes

Sutton and Graves, Fay and Riddel correlations:

$$q_{conv}^{w} = f\left[\sqrt{\left(\frac{du}{dx}\right)_{s}}\right]$$

from Newtonian theory:
$$\left[\left(\frac{du}{dx}\right)_s\right] = \frac{1}{R}\sqrt{\frac{2p-p_\infty}{\rho}}$$

$$q_{conv}^w \propto \frac{1}{\sqrt{R}}$$

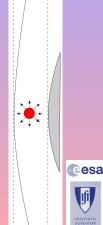
Radiative Fluxes

Optically Thin shock layer:
$$q_{rad}^w = \left(\frac{E\delta}{2}\right)^a$$
 with $\delta \simeq \frac{R}{\rho_s/\rho_\infty}$

$$q_{rad}^{w} \propto R$$

Requirements for minimizing convective and radiative heat fluxes are mutually exclusive

 $[^]a$ E: radiated power, half goes upstream, half to the wall. δ is the shock standoff. s: shock





Stagnation Streamline flux dependence on entry speed

Convective fluxes

$$q_{conv}^w pprox 1/2
ho_\infty u_\infty^3 \mathrm{St}^a$$

 $q_{conv}^w \propto u_\infty^3$

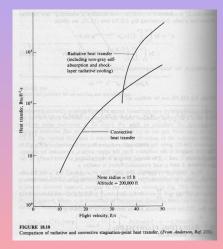
Radiative Fluxes

$$T_s = \frac{u_{\infty}^2}{2C_{p_s}};$$

$$q_{rad}^w = \sigma T_s^4 = \frac{u_{\infty}^8}{(2C_{p_s})^4}$$

$$q_{rad}^w \propto u_{\infty}^8$$

Radiation dominates above 10km/s





^aSt: Stanton number

Boltzmann and Goulard Numbers

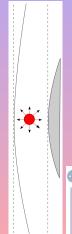
Boltzmann number B_o^{-1} , Radiation/Convection ratio:

$$B_o^{-1} = \frac{q_{rad}}{q_{conv}} = \frac{\sigma T^4}{\rho u C_p T}$$

Infinite slab approximation^a. We also have $C_pT \cong u_{\infty}/2$.

Goulard Number **Γ**, Radiative cooling parameter

$$\Gamma = \frac{2q_{rad}^w}{q_{conv}^w} = \frac{2q_{rad}^w}{1/2\rho_\infty u_\infty^3}$$







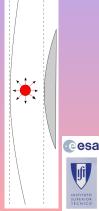
σ: Stefan-Boltzmann constant

^ahalf the radiated power goes upstream, half to the wall

Optically Thin and Optically Thick Limiting Cases

- $\Gamma_n = \frac{4\sigma T_s^4 \alpha \delta}{\rho_{\infty} \mu_{\infty} h_s}$ Optically Thin:
- $\Gamma_k = \frac{16\sigma T_s^4 \alpha}{3\sigma_{ss} \mu_s h}$ Optically Thick^a:
- \circ $\Gamma < 10^{-3}$: radiation is not important
- $10^{-3} < \Gamma < 10^{-2}$: radiation is important but coupling is not necessary
- $\Gamma > 10^{-2}$: coupling of the radiation to the flowfield is necessary

The absorption coefficient is related to the optical transmissivity such that $T = \exp(-\alpha \delta)$. Transmissivity goes from 100% (optically thin) to 0% (optically thick).





aknown as the Rosseland limit

Radiative Transfer Regimes

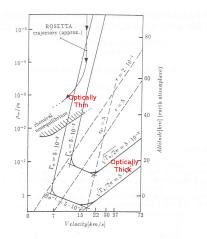
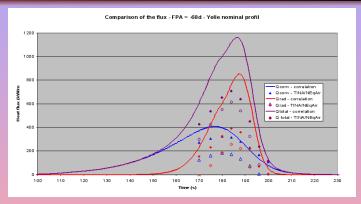


Figure 2: Radiative transfer regimes for a blunt body of 1 ft nose radius, taken from [2]



Sample Correlated Heat Fluxes for the Huygens Entry



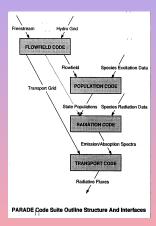
Correlated and simulated convective heat fluxes for the Huygens entry

Engineering correlations allow a first sampling of the spacecraft shape and the selection of an appropriate descent trajectory. Then CFRD simulations can be carried out for specific trajectory points



Computational Fluid Radiative Dynamics Simulations

- Development of radiative databases providing the spectral-dependent emission ε_{ν} and absorption $\alpha(\nu)$ coefficients for any arbitrary state of the plasma
- Accounting for bound, bound–free (photodissociation, photoionization, photodetachment) and free-free (Bremstrahlung) transitions
- bound-bound transitions include atomic, diatomic and polyatomic transitions
- Radiative transfer equation is then solved over the computational domain

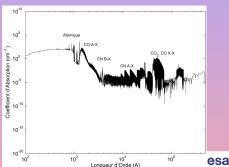






Development of Spectral Databases

- atomic and polyatomic transitions typically simulated from external radiative databases (NIST, TopBase, HITRAN)
- diatomic transitions databases are explicitly obtained using appropriate quantum-mechanics models
- continuum radiation calculated from published absorption cross-sections (e.g. TopBase for atomic photoionization), or from semi-empirical to exact cross-sections for molecular continuum cross-sections



Absorption Coefficient for a 97%CO₂-3%N₂ Plasma in Thermochemical Equilibrium at 5000K and 1bar



- "Collection" of lines which correspond to the overall quantum-allowed radiative transitions between the internal levels of an atom/molecule.
- Selection rules define the quantum-allowed transitions, which must respect angular and spin momentum conservation for atoms and molecules.
- Three key parameters:
 - 1) Line position considering Planck's Law: $\nu = E_u E_l/hc$
 - 2) Line intensity: $I_{\nu} = N_u A_{ul} \Delta E_{ul}$
 - 3) Line profile: $F(\nu nu_0)$, Voigt (sum of a Lorentz & Gaussian profile).
- Radiative spectra obtained through the superposition of these overall



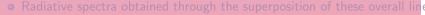


- "Collection" of lines which correspond to the overall quantum-allowed radiative transitions between the internal levels of an atom/molecule.
- Selection rules define the quantum-allowed transitions, which must respect angular and spin momentum conservation for atoms and molecules.
- Three key parameters:
 - 1) Line position considering Planck's Law: $\nu = E_u E_l/hc$;
 - 2) Line intensity: $I_{\nu} = N_u A_{ul} \Delta E_{ul}$
 - 3) Line profile: $F(\nu nu_0)$, Voigt (sum of a Lorentz & Gaussian profile).
- Radiative spectra obtained through the superposition of these overall li

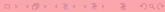




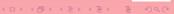
- "Collection" of lines which correspond to the overall quantum-allowed radiative transitions between the internal levels of an atom/molecule.
- Selection rules define the quantum-allowed transitions, which must respect angular and spin momentum conservation for atoms and molecules.
- Three key parameters:
 - 1) Line position considering Planck's Law: $\nu = E_u E_l/hc$;
 - 2) Line intensity: $I_{\nu} = N_u A_{ul} \Delta E_{ul}$;
 - 3) Line profile: $F(\nu nu_0)$, Voigt (sum of a Lorentz & Gaussian profile)







- "Collection" of lines which correspond to the overall quantum-allowed radiative transitions between the internal levels of an atom/molecule.
- Selection rules define the quantum-allowed transitions, which must respect angular and spin momentum conservation for atoms and molecules.
- Three key parameters:
 - 1) Line position considering Planck's Law: $\nu = E_u E_l/hc$;
 - 2) Line intensity: $I_{\nu} = N_u A_{ul} \Delta E_{ul}$;
 - 3) Line profile: $F(\nu nu_0)$, Voigt (sum of a Lorentz & Gaussian profile).
- Radiative spectra obtained through the superposition of these overall lines



Key Parameters

The fundamental equation for intensity

$$I_{\nu} = N_{u}A_{ul}\Delta E_{ul}F(\nu - \nu_{0})$$

can be decoupled in the following variables:

- N_u : Level populations
 - Either a Boltzmann equilibrium distribution, either through Collisional-Radiative nonequilibrium models
- ullet A_{ul} : Transition probabilities (Einstein Coefficients)
 - From "ab-initio" or measured transition moments
- ΔE_{ul} : Level energies:

Fitting and extrapolation of experimentally determined data

• $F(\nu - \nu_0)$: Line profile:

Voigt profiles accounting for Doppler and Collisional broadening (depends on the lo conditions of the plasma)



@esa

Key Parameters

The fundamental equation for intensity

$$I_{\nu} = N_{u}A_{ul}\Delta E_{ul}F(\nu - \nu_{0})$$

can be decoupled in the following variables:

- N_u: Level populations:
 Either a Boltzmann equilibrium distribution, either through Collisional-Radiative nonequilibrium models
- A_{ul}: Transition probabilities (Einstein Coefficients):
 From "ab-initio" or measured transition moments
- ΔE_{ul} : Level energies: Fitting and extrapolation of experimentally determined data
- $F(\nu \nu_0)$: Line profile:

 Voigt profiles accounting for Doppler and Collisional broadening (depends on the local conditions of the plasma)

esa

Rotational-Vibrational Level Energies of Diatomic Molecules

$$E_{e,v,J} = T_e + G(v) + B_v(J)$$

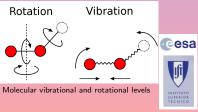
$$= T_e + \omega_e (v + 1/2) - \omega_e x_e (v + 1/2)^2 + \omega_e y_e (v + 1/2)^3 + \dots$$

$$+ \left[B_e - \alpha_e (v + 1/2) + \gamma_e (v + 1/2)^2 + \dots \right] [J(J+1)]$$

$$- \left[D_e + \beta_e (v + 1/2) + \dots \right] [J(J+1)]^2 + \dots$$

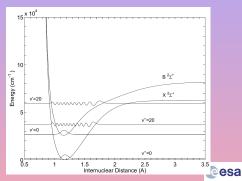
In the compact Dunham matrix form (strictly valid only for $^{1}\Sigma$ states):

$$E_{e,v,J} = \sum_{i,j} Y_{ij} (v + 1/2)^i [F(J)]^j,$$



Potential Reconstruction Methods

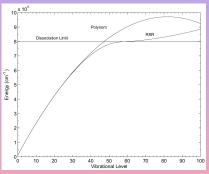
- Potential reconstruction methods allow determining the radial wavefunction for the molecular vibrational levels.
- They also incidentally allow more accurate representations of near-dissociative levels, where polynomial expansions are no longer valid.



Sample RKR calculation for the CN Violet system

One Sample Application

- Calculation of the vibrational levels for the $N_2(X^1\Sigma)$ ground state.
- Traditional polynomial expansions predict v_{max}=46.
- A more rigorous RKR potential reconstruction method yields v_{max}=61.



 $N_2(X^1\Sigma)$ Level energies calculated using a second order polynomial expansion, and the RKR method





Fine-structure Effects (1/4)

- Fine-strucure effects like spin splitting and Λ-Doubling for homonuclear molecules, split one single line into multiplet lines with energies very close one to another.
- Nuclear momentum is named as Σ , Π , Δ , etc..., for $\Lambda = 0, 1, 2$
- The level energies expressions for spin splitted lines are summarized next





Fine-structure Effects (2/4)

• Singlet States with $\Lambda \neq 0$

$$F_{\nu}(J) = B_{\nu}(J(J+1)) + (A_{\nu} - B_{\nu})\Lambda^{2}$$

Doublet States

$$F_{3/2}(J \ge 1) = B_v \begin{bmatrix} (J + \frac{1}{2})^2 - \Lambda^2 \\ -\frac{1}{2} \left(4 \left(J + \frac{1}{2} \right)^2 + Y_v (Y_v - 4) \Lambda^2 \right)^{\frac{1}{2}} \end{bmatrix} - D_v J^4$$

$$F_{1/2}(J \ge 0) = B_v \begin{bmatrix} (J + \frac{1}{2})^2 - \Lambda^2 \\ +\frac{1}{2} \left(4 \left(J + \frac{1}{2} \right)^2 + Y_v (Y_v - 4) \Lambda^2 \right)^{\frac{1}{2}} \end{bmatrix} - D_v (J + 1)^4$$
 esa

Fine-structure Effects (3/4)

³Σ Triplet States

$$\begin{split} ^{3}\Sigma_{2}(J \geq 2) &= B_{\nu}(J(J+1)) - D_{\nu}(J(J+1))^{2} - \left(\lambda_{\nu} - B_{\nu} + \frac{1}{2}\gamma_{\nu}\right) \\ &- \left[\left(\lambda_{\nu} - B_{\nu} + \frac{1}{2}\gamma_{\nu}\right)^{2} + 4J(J+1)\left(B_{\nu} - \frac{1}{2}\gamma_{\nu}\right)^{2}\right]^{\frac{1}{2}} \\ ^{3}\Sigma_{1}(J \geq 1) &= B_{\nu}(J(J+1)) - D_{\nu}(J(J+1))^{2} \\ ^{3}\Sigma_{0}(J \geq 0) &= B_{\nu}(J(J+1)) - D_{\nu}(J(J+1))^{2} - \left(\lambda_{\nu} - B_{\nu} + \frac{1}{2}\gamma_{\nu}\right) \\ &+ \left[\left(\lambda_{\nu} - B_{\nu} + \frac{1}{2}\gamma_{\nu}\right)^{2} + 4J(J+1)\left(B_{\nu} - \frac{1}{2}\gamma_{\nu}\right)^{2}\right]^{\frac{1}{2}} \end{split}$$





Fine-structure Effects (4/4)

³Π Triplet States

$$\label{eq:definition} \begin{split} ^3\Pi_2(J\!\geq\!2) &= B_v \left[\begin{array}{c} J(J+1) - \sqrt{y_1 + 4J(J+1)} \\ -\frac{2}{3}\frac{y_2 - 2J(J+1)}{y_1 + 4J(J+1)} \end{array} \right] - D_v \left(J - \frac{1}{2}\right)^4 \\ ^3\Pi_1(J\!\geq\!1) &= B_v \left[J(J+1) + \frac{4}{3}\frac{y_2 - 2J(J+1)}{y_1 + 4J(J+1)} \right] - D_v \left(J + \frac{1}{2}\right)^4 \\ ^3\Pi_0(J\!\geq\!0) &= B_v \left[\begin{array}{c} J(J+1) + \sqrt{y_1 + 4J(J+1)} \\ -\frac{2}{3}\frac{y_2 - 2J(J+1)}{y_1 + 4J(J+1)} \end{array} \right] - D_v \left(J + \frac{3}{2}\right)^4 \end{split}$$

with

$$y_1 = Y_v(Y_v - 4) + \frac{4}{3}$$
 $y_2 = Y_v(Y_v - 1) - \frac{4}{9}$ $Y_v = \frac{A_v}{B_v}$

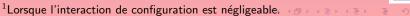




Selection Rules for Atoms

	Transitions E1	Transitions M1	Transitions E2	
Tous types de couplages				
1	$\Delta J = 0, \pm 1$ (sauf 0 \leftrightarrow 0)	$\Delta J = 0, \pm 1$ (sauf 0 \leftrightarrow 0)	$\Delta J = 0, \pm 1, \pm 2$ (sauf $0 \leftrightarrow 0$, $\frac{1}{2} \leftrightarrow \frac{1}{2}, 1 \leftrightarrow 1$)	
2	$\Delta M = 0, \pm 1$ (sauf $0 \leftrightarrow 0$ lorsque $J = 0$)	$\Delta M = 0, \pm 1$ (sauf $0 \leftrightarrow 0$) lorsque $J = 0$)	$\Delta M = 0, \pm 1, \pm 2$	
3	changement de parité	parité identique	parité identique	
41	transition d'un électron avec $\Delta I=\pm 1$, Δn arbitraire	pas de changement dans la configuration électronique, soit pour tous les électrons: $\Delta l = 0, \ \Delta n = 0$	pas de changement dans la configuration électronique, ou bien pour un électron: $\Delta l = 0, \pm 2,$ Δn arbitraire	
		Couplage L-S		
5	$\Delta S = 0$	$\Delta S = 0$	$\Delta S = 0$	
6	$\Delta L = 0, \pm 1$ (sauf 0 \leftrightarrow 0)	$\Delta L = 0$, $\Delta J = \pm 1$	$ \Delta L = 0, \pm 1, \pm 2 $ (sauf $0 \leftrightarrow 0$, $0 \leftrightarrow 1$)	





Selection Rules for Molecules

transition entre niveaux de rotation	$\Delta J = 0, \pm 1$ (sauf 0 \leftrightarrow 0)
parité des niveaux de rotation	$+ \leftrightarrow -$ permis $+ \leftrightarrow +, - \leftrightarrow -$ interdits
branches de rotation $Q(\Delta J=0)$	$e \leftrightarrow f$ permis $e \leftrightarrow e, f \leftrightarrow f$ interdits
branches de rotation $P, R(\Delta J = \pm 1)$	$e \leftrightarrow e, f \leftrightarrow f$ permis $e \nleftrightarrow f$ interdits
molecules homonucleaires	$s \leftrightarrow s, a \leftrightarrow a$ permis $s \nleftrightarrow a$ interdits
noyaux de même charge	$g \leftrightarrow u$ permis $g \leftrightarrow g, u \leftrightarrow u$ interdits





Transition Probabilities (1/2)

Transition probability A_{ul} decomposed into vibronic and rotational product

$$A_{ul} = A_{e^{\prime\prime}v^{\prime\prime}}^{e^{\prime}v^{\prime}} \cdot A_{\Lambda^{\prime\prime}J^{\prime\prime}}^{\Lambda^{\prime}J^{\prime}}$$

with

$$A_{e''v''}^{e'v'} = \frac{64\pi^4 \overline{\nu}^3}{3hc^3} \frac{\left(2 - \delta_{0,\Lambda'+\Lambda''}\right)}{\left(2 - \delta_{0,\Lambda'}\right)} \left(R_e^{v'v''}\right)^2$$

and

$$\left(R_{\mathsf{e}}^{v'v''}\right)^2 \cong \frac{\sum \left(R_{\mathsf{e}}^{v'v''}\right)^2}{(2 - \delta_{0,\Lambda'+\Lambda''})(2S+1)}$$

The vibronic transition moment being obtained from the integration of the electronic transition moment $R_e(r)$ and the upper and lower states wavefunctions

$$\left(R_e^{v'v''}\right)^2 = \left(\int \psi_{v'}(r)R_e(r)\psi_{v''}(r)dr\right)^2$$



Transition Probabilities (2/2)

The rotational transiton probability is given by the Hönl-London factors

$$A_{\Lambda^{\prime\prime}J^{\prime\prime}}^{\Lambda^{\prime}J^{\prime\prime}} = \frac{S_{\Lambda^{\prime\prime}J^{\prime\prime}}^{\Lambda^{\prime}J^{\prime\prime}}}{2J^{\prime}+1}$$

which depend on the type of rotation-electronic motion coupling (Hund Case), and the type of electronic transition $({}^{n}\Lambda \leftrightarrow {}^{n}\Lambda)$. We use the normalization rule

$$\sum_{J''} S_{\Lambda''J''}^{\Lambda'J'}(J') = (2J'+1)$$

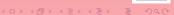
and we may then write

$$A_{ul} = \frac{64\pi^4 \overline{\nu}^3}{3hc^3} \frac{\sum \left(R_e^{v'v''}\right)^2}{(2 - \delta_{0,\Lambda'})(2S+1)} \frac{S_{\Lambda''J''}^{\Lambda'J'}}{2J'+1}$$



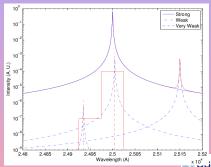
Voigt Lineshape Calculation Method

- Line broadening mechanisms from Doppler or collision effects (Lorentz lineshape).
- Objective: To calculate the most accurate Voigt lineshape (convolution of Doppler and Lorentz lineshapes) utilizing a minimum number of points.
- Input parameters: line position, emission/absorption coefficient, Doppler/Lorentz FWHM.
- Starting point: Analytical expression of Whiting, updated by Olivero (JQSRT, Vol. 17, 1977, pp. 233).
- Definition of low-resolution lines (5 to 11 grid points) and high-resolution lines (typically more than 20 points).

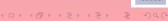


Definition of Strong and Weak Lines

- Definition of strong, weak, and very weak lines.
- In the "pseudo-continuum" approach, only strong lines and uncovered weak lines are calculated explicitly. Other lines are added as a continuum.

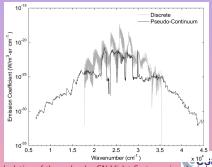


Sample strong, weak, and very weak lines (with thresholds 10° 10°)



Sample Calculation for the CN Violet System

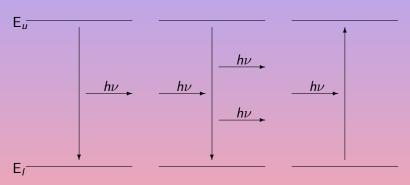
- Here, only the strong lines for diagonal transitions are explicitly calculated.
- The "pseudo-continuum" extends below.
- Significant savings in calculation times and spectral grid sizes can be achieved (Lino da Silva, JQSRT 2007)



Calculation of the molecular CN Violet System using the hybric line-by-line/pseudo-continuum approach.



Elementary Radiative Processes



spontaneous emission induced emission

$$\frac{\partial N_u}{\partial t} = -N_u A_{ul}$$

$$\frac{\partial N_u}{\partial t} = -N_u$$

$$I_{
u}$$
 -

$$\frac{\partial N_u}{\partial t} = -N_u A_{ul} \qquad \frac{\partial N_u}{\partial t} \quad = -N_u B_{ul} u_{\nu} \quad \frac{\partial N_l}{\partial t} = -N_u B_{ul} u_{\nu}$$

absorption



The Line-by-Line Method: Level Energies
The Line-by-Line Method: Transition Probabilities
The Line-by-Line Method: Lineshapes
Exact Radiative Transfer Methods

Derivation of the Radiative Transfer Equation (RTE) (1/2)

Summing the three processes we have

$$\frac{\partial N_u}{\partial t} = -N_u A_{ul} + [N_u B_{ul} - N_u B_{ul}] u_{\nu}$$

In Radiative equilibrium the net variation is 0, and radiation is given by the Planck Blackbody Law

$$u_{\nu}^{\mathrm{o}}(T) = \frac{8\pi h \nu^3}{c^3} \left[\exp\left(-\frac{h\nu}{k_B T}\right) - 1 \right]^{-1}$$

we have

$$g_I B_{Iu} = g_u B_{uI}$$
$$\frac{A_{uI}}{B_{uI}} = \frac{8\pi h \nu^3}{c^3}$$





Derivation of the Radiative Transfer Equation (RTE) (2/2)

Integrating the expressions of the previous slide in volume from we obtain the classical RTE equation:

$$\cos\theta \frac{dL_{\nu}}{dz} = \varepsilon_{\nu} - \alpha_{\nu} L_{\nu}$$

with

$$\varepsilon_{\nu} = \frac{n_{u}A_{ul}h\nu}{4\pi}$$
$$\alpha(\nu) = \left(n_{u} - \frac{g_{u}}{g_{l}}n_{l}\right)B_{ul}\frac{h\nu}{c}$$

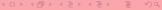
which becomes the Beer-Lambert Law in 1D coordinates:

$$\frac{dI_{\nu}}{dI} = \varepsilon - \alpha(\nu)I_{\nu}$$

and after integration:

$$I_{\nu} = \frac{\varepsilon}{\alpha(\nu)} [1 - \exp(-\alpha(\nu)I)]$$





Detailed Balancing Principle for Radiation

Bound-Bound Transitions

$$\frac{\varepsilon_{\nu}}{\alpha_{\nu}} = \frac{2h\nu^3}{c^2} \left(\frac{g_u n_l}{g_l n_e} - 1 \right)^{-1}$$

Bound-Free Transitions

$$\frac{\sigma_{bf}(\nu)}{\sigma_{fb}(\nu)} = \frac{1}{2} \left(\frac{m_e v_e c}{h \nu} \right)^2 \frac{g_+ g_e}{g_n}$$

Free-Free Transitions

$$rac{arepsilon_{
u}}{lpha_{
u}} = rac{2h
u^3}{c^2} \left[\exp\left(rac{h
u}{k_B T_e}
ight) - 1
ight]^{-1}$$





Detailed Balancing Principle for Radiation

Bound-Bound Transitions

$$\frac{\varepsilon_{\nu}}{\alpha_{\nu}} = \frac{2h\nu^3}{c^2} \left(\frac{g_u n_l}{g_l n_e} - 1 \right)^{-1}$$

Bound-Free Transitions

$$\frac{\sigma_{bf}(\nu)}{\sigma_{fb}(\nu)} = \frac{1}{2} \left(\frac{m_e v_e c}{h \nu} \right)^2 \frac{g_+ g_e}{g_n}$$

Free-Free Transitions

$$\frac{\varepsilon_{\nu}}{\alpha_{\nu}} = \frac{2h\nu^{3}}{c^{2}} \left[\exp\left(\frac{h\nu}{k_{B}T_{e}}\right) - 1 \right]^{-1}$$





Detailed Balancing Principle for Radiation

Bound-Bound Transitions

$$\frac{\varepsilon_{\nu}}{\alpha_{\nu}} = \frac{2h\nu^3}{c^2} \left(\frac{g_u n_l}{g_l n_e} - 1 \right)^{-1}$$

Bound-Free Transitions

$$\frac{\sigma_{bf}(\nu)}{\sigma_{fb}(\nu)} = \frac{1}{2} \left(\frac{m_e v_e c}{h \nu} \right)^2 \frac{g_+ g_e}{g_n}$$

Free-Free Transitions

$$\frac{\varepsilon_{\nu}}{\alpha_{\nu}} = \frac{2h\nu^3}{c^2} \left[\exp\left(\frac{h\nu}{k_B T_e}\right) - 1 \right]^{-1}$$



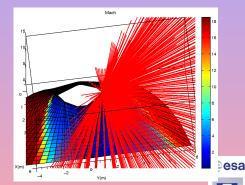


The Line-by-Line Method: Level Energies
The Line-by-Line Method: Transition Probabilities
The Line-by-Line Method: Lineshapes
Exact Radiative Transfer Methods

Ray-Tracing Methods for Space-Related Heat Transfer Analysis

 Ray-Tracing: An exact method for determining the quantities of photons which irradiate a surface.

$$q_{
u} = \int_{-\pi/2}^{\pi/2} \int_{0}^{\pi} I_{
u}(\theta, \phi) cos\theta \sin\theta d\theta d\phi$$
 $I_{
u} = rac{arepsilon}{lpha'} [1 - \exp(-lpha I(heta))]$



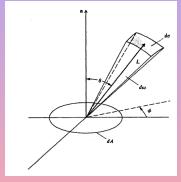
Ray-tracing considers full 3D geometries, with the possibility of simple 2D/1D slab geometries.



Ray-Tracing Methods for Space-Related Heat Transfer Analysis

 Ray-Tracing: An exact method for determining the quantities of photons which irradiate a surface.

$$q_
u = \int_{-\pi/2}^{\pi/2} \int_0^\pi I_
u(heta,\phi) cos heta \sin heta d heta d\phi$$
 $I_
u = rac{arepsilon}{lpha'} [1 - \exp(-lpha I(heta))]$





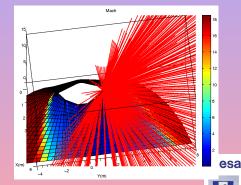
• Ray-tracing considers full 3D geometries, with the possibility of simple 2D/1D slab geometries.



Ray-Tracing Methods for Space-Related Heat Transfer Analysis

 Ray-Tracing: An exact method for determining the quantities of photons which irradiate a surface.

$$q_
u = \int_{-\pi/2}^{\pi/2} \int_0^\pi I_
u(heta,\phi) cos heta \sin heta d heta d\phi$$
 $I_
u = rac{arepsilon}{lpha'} [1 - \exp(-lpha I(heta))]$



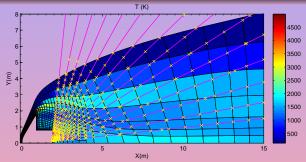
 Ray-tracing considers full 3D geometries, with the possibility of simpler 2D/1D slab geometries.

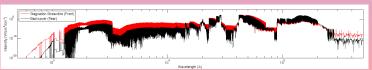




The Line-by-Line Method: Level Energies
The Line-by-Line Method: Transition Probabilities
The Line-by-Line Method: Lineshapes
Exact Radiative Transfer Methods

Ray-Tracing Methods for Space-Related Heat Transfer Analysis







Complex flow geometries with millions of molecular spectral lines

Fitan Entry: Huygens High-Speed Earth Reentry: Phoebus Mars Entry: PHOENIX and EXOMARS Ground Plasma Facilities

Case Studies





Titan Entry: Huygens High-Speed Earth Reentry: Phoebus Mars Entry: PHOENIX and EXOMARS Ground Plasma Facilities

Huygens Titan Entry (2005)

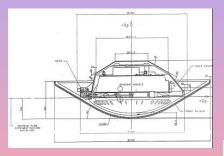
• 60 half angle blunted cone

Base diameter: 2.7 m

Nose radius: 1.25 m

Entry module mass: 318.62 kg

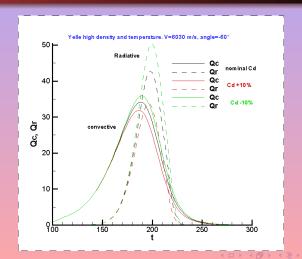
 Aerodynamic databases developed by EADS between 1991 and 1995.





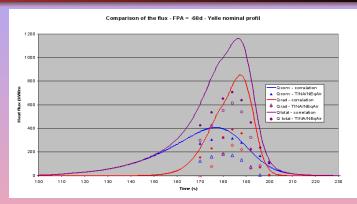


Huygens Heat Fluxes: Dispersions associated to Cd uncertainties





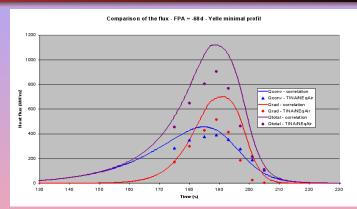
Huygens Heat Fluxes: Nominal Yelle Atmospheric Profile



- Titan Composition: 95% N₂-5% CH₄
- Important Radiator species CN produced in the shock layer.
 correlations do not work anymore.



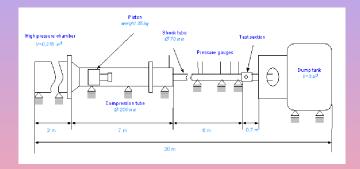
Huygens Heat Fluxes: Nominal Yelle Atmospheric Profile



- Titan Composition: 95% N₂-5% CH₄
- Important Radiator species CN produced in the shock layer.
 correlations do not work anymore.



Validation of Aerothermodynamic Databases: Shock-Tubes Experiments



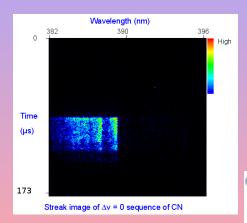
 TCM2 Shock-Tube at Marseilles, France, was utilized for validating the CFRD models used for Huygen's Entry



Acquisition Results: CN spectral time-resolved picture

Shot conditions:

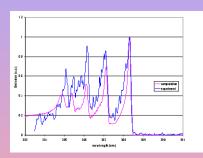
- Shock Tube Classical mixture p_{shock}=200 Pa
- Shock velocityv_{shock}=5680 m/s



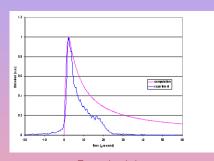




40 Pa test rebuilding, Boltzmann



Non-equilibrium zone, 1s integration

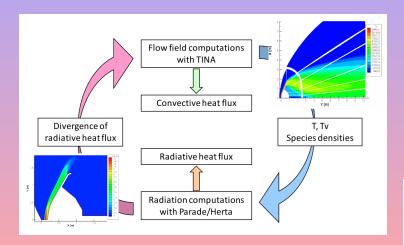


Temporal evolution

Validation of Aerothermal databases against simpler (1D, time-dependent) representative flow conditions



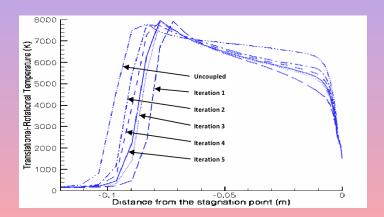
Coupled CFD-Radiatve Simulations of Huygens Entry







Stagnation Streamline Temperatures Variation During CFD-Radiation Iterations







Spectral Convergence

Table 1: Influence of number of points for radiative heat flux

		Without Al	osorption	With Absorption		
Nb points	Resolution (pt/Å)	Q rad kW/m2	Variation %	Q rad kW/m2	Variation %	
5 000	0.28	2091.33	+0.05	1773.38	+30.58	
50 000	2.78	2091.00	+0.03	1603.38	+18.06	
100 000	5.56	2090.96	+0.03	1535.54	+13.07	
200 000	11.1	2090.59	+0.01	1488.07	+9.57	
1 800 000	100	2090.28	-	1358.08	-	

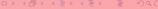




Influence of Radiation and Radiation Coupling

Radiative heat flux		W ithout coupling	W ith coupling	
W ithout Absorption	k W /m 2	813.82	516.82	
W ith Absorption	k W /m 2	558.41	401.87	
V a ria tio n		W ithout coupling	W ith coupling	
W ithout Absorption	%		-36%	
With Absorption	%	-31%	-51%	





Phoebus High-Speed Entry Demonstrator

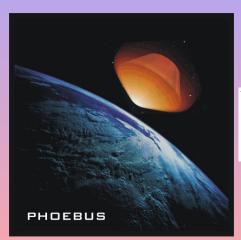


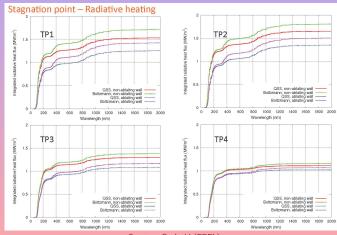
Table 9.2: Phoebus simulation trajectory points and specifics of the corresponding freestream

Name	Time	Altitude	$\rho_{\infty}~(\mathrm{kg/m^3})$	<i>T</i> _∞ (K)	p_{∞} (Pa)	u_{∞} (m/s)	Mach
TP1	18.4	64981	1.64e-4	233.3	10.96	10916	35.65
TP2	21.8	55449	4.23e-4	254.0	30.96	10044	32.04
TP3	24.1	49464	1.10e-3	270.6	85.28	9518	28.86
TP4	26. 0	45004	2.00e-3	264.2	149.10	8456	25.95





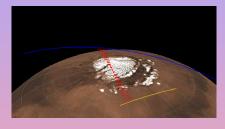
Coupled Radiative Calculations with Ablation and Boltzmann Nonequilibrium Effects





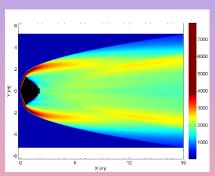
Mars EXPRESS Observation of the PHOENIX Entry

- ESA Mars EXPRESS Orbiter provided support for PHOENIX 2008 Mars Entry
- Mars EXPRESS Tracked PHOENIX Entry with his onboard instrumentation (First Attempt at tracking an Entry from an Onboard Satellite).

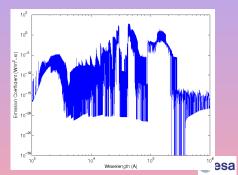


- CFRD simulations prior to entry predicted the IR trail to be the most emissive.
- SPICAM VUV Camera and HRSC Visible Camera tracked the Entry IR Fourier Spectrometer could not be turned on due to power budget constraints.

CFRD Simulations of PHOENIX Entry



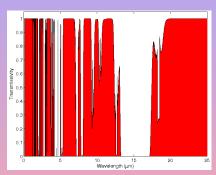
PHOENIX Temperature Profiles, t=203s



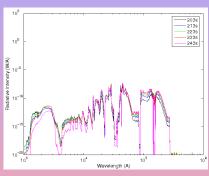
Sample spectrum of the PHOENIX Plume

Titan Entry: Huygens High-Speed Earth Reentry: Phoebus Mars Entry: PHOENIX and EXOMARS Ground Plasma Facilities

Radiative Transfer Towards Mars EXPRESS



Optical path Transmissivity



Raddiation collected by one pixel of the Mars EXPRESS instrumentation

Radiation in the VUV-Visible region was not detected, IR radiation was predicted to be detected if the instrument had been switched on



Spectral Database for CO₂–N₂ Mixtures

- CO₂ Infrared
- CO Infrared
- CO 4⁺
- CO 3⁺
- CO Angstrom
- CO Triplet
- CN Violet
- CN Red
- C₂ Swan
- C₂ Phillips
- C₂ Mulliken
- C₂ Deslandres-D'Azambuia
- C₂ Ballik–Ramsay

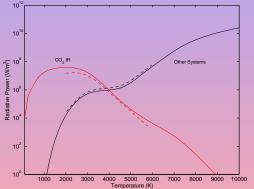
- O₂ Sch.–Runge
- O₂ Sch.-Runge Cont.
- No 1+
- $N_2 2^+$
- NO Gamma
- NO Beta
- NO Delta
- NO Epsilon
- NO Beta
- C Atomic
- C Photoionization
- N Atomic
- N Photoionization

- O Atomic
- O Photoionization
- C- Photodetachment
- N⁻ Photodetachment
- O- Photodetachment
- CO₂ Photoionization N₂ Photoionization
- O₂ Photoionization
- CN Photoionization CO Photoionization
- NO Photoionization of





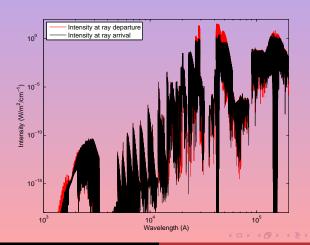
Radiative Power for CO₂–N₂ Mixtures: Comparison With Other Spectral Databases



Comparison of the overall temperature dependent radiative power of CO_2 IR radiation (red) and for the other radiative systems (black) for an atmospheric pressure, Martian-type CO_2 – N_2 plasma. Comparison is carried for the SPARTAN code database (full lines) and the EM2C database (dotted lines).



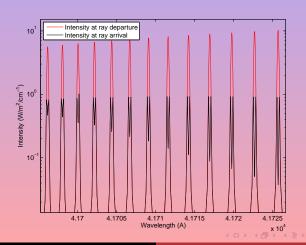
Example of a Ray Departing from the Afterbody Plume; PH(1/2)





Ittan Entry: Huygens
High-Speed Earth Reentry: Phoebus
Mars Entry: PHOENIX and EXOMARS
Ground Plasma Facilities

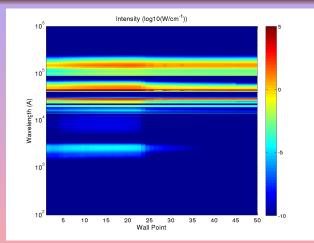
Example of a Ray Departing from the Afterbody Plume; PH(2/2)







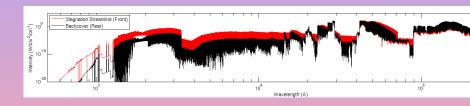
Spectral Distribution of the Wall Fluxes; PH





 CO_2 IR radiation is dominant, with traces of CO 4^+ , CO 3^+ , and CO Angstrom in the forebody

Comparison of Stagnation Streamline and Backcover Shoulder Spectra; PH

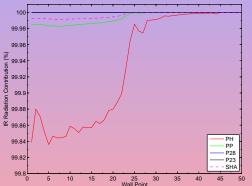


- VUV-Visible radiation higher for the stagnation streamline points
- For both points, CO₂ radiation spectral intensity is several orders of magnitude above Visible-VUV radiation





Contribution of Radiative Fluxes above $1\mu\mathrm{m}$ to the Overall Radiative Power; Large Spacecraft Configuration

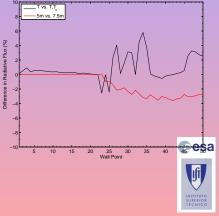


Values for the smaller spacecraft configuration are similar. Other studies in the scope of the ESA TC3 testcase confirm such findings for CO_2 – N_2 mixtures (CN and C_2 radiation less than 3% overall in the stagnation streamline point.

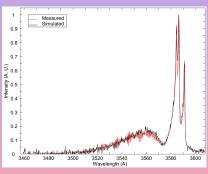


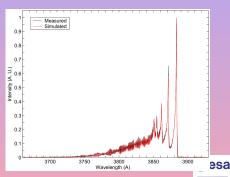
Sensitivity Studies

- Ray-tracing calculations carried for peak conductive heating (PH; Tv/T 1.2) either considering (T,Tv)or just (T).
- Ray-tracing calculations carried at 2.8km/s (P28) with a 5m and a 7.5m afterbody flow.
- Influence of thermal nonequilibrium less than 5% on wall fluxes, and enough backflow is accounted for (3% diff. max).



A Careful Tailoring of Spectroscopic Databases Allows Very Good Fits of Equilibrium Radiation





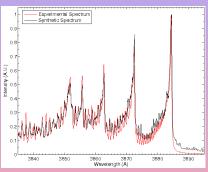
Best-fit to a measured CN Violet Spectrum ($\Delta \nu = 1$)

Best-fit to a measured CN Violet Spectrum ($\Delta v =$

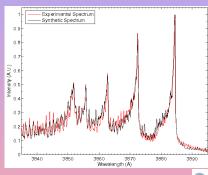
Spectra measured in equilibrium conditions in an ICP torch (97% CO_2 -3% N_2 gas)



But Radiation is not Always Boltzmann!

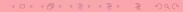


Fitting of the CN Violet system, assuming T_r =10000K and a Boltzmann vibrational distribution

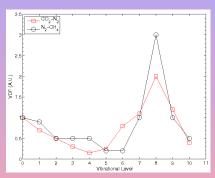


Fitting of the CN Violet system, assuming T_r=2700K **esa**

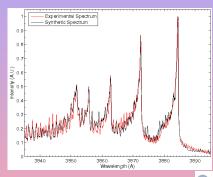
Fitting of a strongly nonequilibrium CN Violet Spectra obtained in a Supersonic Arc-Jet for a Titan-type (95% N_2 –5% CH_4 gas)



But Radiation is not Always Boltzmann!



non-Boltzmann vibrational distribution Function



Fitting of the CN Violet system, assuming T_r =270 \Re esa and a non-Boltzmann vibrational distribution

Fitting of a strongly nonequilibrium CN Violet Spectra obtained in a Supersonic Arc-Jet for a Titan-type (95% N_2 –5% CH₄ gas)

